Thermodynamics and tunneling spectroscopy in the pseudogap regime of the boson fermion model

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Motivated by the STM experimental data on $Bi_2Sr_2CaCU_2O_{8+x}$ which indicate the tunneling conductance asymmetry $\sigma(-V) \neq \sigma(V)$, we report that such a behavior can be explained in terms of the boson fermion model. It has been shown in the recent studies, based on various selfconsistent techniques to capture the many-body effects, that the low energy spectrum of the boson fermion model is featured by an appearance of the pseudogap at $T^* > T_c$. We argue that the pseudogap structure has to exhibit a particle-hole asymmetry. This asymmetry may eventually depend on the boson concentration.

1. Introduction

Recently there was a considerable amount of studies of the pseudogap phenomenon observed in a variety of experiments on the high temperature superconductors (HTSC) [1]. There are two main theoretical interpretations which are presently widely considered in the literature: (i) the pseudogap as a precursor of the emerging pairing fluctuations, and (ii) the pseudogap understood in terms of some new (hidden) ordering taking place in a vicinity of the superconducting phase. Some selective overview can be found e.g. in the recent monograph [2].

Among theoretical attempts to explain the pseudogap effect of HTSC materials there is a model of itinerant electrons or holes which coexist and interact with the local bound pairs (hard-core bosons) [3]. It is worth mentioning, that the pseudogap has been foreseen within this boson fermion (BF) model a long time before the convincing experimental data became available (see the last paragraph in section IV of the Ref. [4]).

Pseudogap phase of the BF model is a manifestation of the pairing-wise correlations which start to appear in a system when the transition temperature T_c is approached from above (the precursor type interpretation). On a microscopic basis it means that below a certain temperature T^* fermions start to couple into the pairs. These are, however, weakly ordered in phase due to the small superfluid stiffness. The phase coherence sets in at a sufficiently low temperature $T_c \leq T^*$ and then the true superconducting transition occurs. Presence of the incoherent ($T^* < T < T_c$) or the coherent ($T_c \geq T$) fermion pairs is accompanied by either the pseudogap or the true superconducting gap formed around the Fermi energy ε_F.

In general, some advanced methods of the many body theory are required to explore a pseudogap phase within any model. It is because the single-particle and the two-particle correlations are then of equal importance. They should be properly treated taking account of possible feedback effects between both channels in a controlled way. In a context of the BF model such requirements were obtained so far via: a) the selfconsistent perturbative investigation [5,6], b) the dynamical mean field theory [7], and c) the flow equation study [8]. Some alternative way was studied by Micnas *et al* [9] who considered the Kosterlitz-Thouless criterion for determination of the superconducting transition $T_c = T_{KT}$ and identified T^* with the mean field estimate $T_c^{(MF)}$. Authors were able to reproduce qualitatively the Uemura type plots T_c versus ρ_s.

In this short paper we extend our previous study [8] to analyze the pseudogap shape and its variation with temperature. Direct consequences

of the particle-hole asymmetric pseudogap are illustrated on an example of the STM current conductance.

2. Model and the origin of correlations

We consider the BF model which is described by the following Hamiltonian [3,4]

$$\begin{aligned} H^{BF} &= \sum_{i,j,\sigma} \left(t_{ij} - \mu\delta_{i,j}\right) c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_i E_0 b^{\dagger}_i b_i \\ &+ v \sum_i \left(b^{\dagger}_i c_{i\downarrow} c_{i\uparrow} + b_i c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} \right) \end{aligned} \quad (1)$$

where $E_0 = \Delta_B - 2\mu$ and Δ_B is the boson energy, μ is the chemical potential. The second quantization operators $c^{(\dagger)}_{i\sigma}$ refer to the conduction band particles (electrons or holes) and $b^{(\dagger)}_i$ to the composite hard-core bosons (for instance they can represent the trapped electron pairs $b_i = d_{i\downarrow} d_{i\uparrow}$). Itinerant fermions propagate between the lattice sites i and j via the hopping integral t_{ij} whereas bosons are assumed to be infinitely heavy. The hard-core property of bosons means that either 0 or 1 boson is allowed to occupy a given lattice site. This local constraint can be formally expressed [4] through the following semi-bosonic commutation relations $\left[b_i, b^{\dagger}_j\right] = \delta_{i,j}\left(1 - 2b^{\dagger}_i b_i\right)$ and $[b_i, b_j] = 0 = \left[b^{\dagger}_i, b^{\dagger}_j\right]$.

Mechanism of superconductivity and all the other forms of correlations in the BF model (1) are caused by the boson fermion charge exchange potential v. By decaying into the fermion pairs, bosons gain effectively some mobility. If temperature decreases below the critical value T_c then (for $dim > 2$) some fraction of bosons gets "frozen" into the BE condensate $n_0(T) = \frac{1}{N}\left\langle b^{\dagger}_{\mathbf{q}=\mathbf{0}} b_{\mathbf{q}=\mathbf{0}}\right\rangle$. For $n_0(T) \neq 0$, fermions are simultaneously driven into the broken symmetry superconducting state. It can be shown [4,8] that the energy gap in the superconducting fermion subsystem is $v\sqrt{n_0(T)}$.

For temperatures slightly higher than T_c there exist many bosons which occupy the small momenta $\mathbf{q} \sim \mathbf{0}$ states. Because of the interaction $v\sum_{\mathbf{k},\mathbf{q}}\left(b^{\dagger}_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}/2\downarrow} c_{-\mathbf{k}+\mathbf{q}/2\uparrow} + h.c.\right)$, these boson states $|n_{\mathbf{q}}\rangle_B$ are strongly mixed with the fermion states $|n_{\mathbf{k}+\mathbf{q}/2\downarrow}\rangle_F$ $|n_{-\mathbf{k}+\mathbf{q}/2\uparrow}\rangle_F$ and thereby the life time of fermions might be reduced, especially for $|\mathbf{k}| \sim k_F$. In consequence, we expect that the fermion density of states might be suppressed near ε_F.

With the on-site boson fermion interaction given in (1) one can generate only the isotropic gap/pseudogap. Of course, the HTSC materials are characterized by the anisotropic order parameters of the d-wave symmetry with a possible admixture of the s-wave component [10]. To capture this aspect it is enough to introduce the intersite coupling $v_{i,j} b^{\dagger}_i \left(c_{i\downarrow} c_{j\uparrow} + c_{j\downarrow} c_{i\uparrow}\right) + h.c.$ when both, the superconducting gap [9,11,12] and the pseudogap [6] become anisotropic. Here we only discuss the results for the isotropic case but, at a price of more difficult numerical computations, the same procedure can be easily extended to the anisotropic pairing.

3. The effective spectra

In order to determine the effective fermion and boson spectra of the model (1) we utilize the flow equation technique proposed by Wegner [13]. The main idea behind is to disentangle the coupled boson and fermion subsystems via a sequence of canonical transformations $H(l) = e^{-S(l)} H e^{S(l)}$, where l is a continuous parameter. We start at $l = 0$ by putting $H^{BF} \equiv H(0)$, and proceed till $l = \infty$, when we want to obtain $H(\infty) = H^F_{eff} + H^B_{eff}$. All the way, from $l = 0$ to $l = \infty$, we adjust the operator $S(l)$ according to the Wegner's prescription [13]. In practice, disentangling of fermion from boson subsystem can be done within an accuracy of the order v^3 [8]. To simplify the matters we neglect the hard-core constraint and use the pure bosonic relations $\left[b_i, b^{\dagger}_j\right] \simeq \delta_{i,j}$ which should be valid for small boson concentrations $n_B = \left\langle b^{\dagger}_i b_i \right\rangle$.

After the disentangling procedure is finished we obtain the following structure for the boson contribution to the effective Hamiltonian $H^B_{eff} = \sum_{\mathbf{q}}\left(E_{\mathbf{q}} - 2\mu\right)$. The initial boson energy Δ_B is thus transformed into the dispersion $E_{\mathbf{q}}$ which is characterized by the width proportional to v^2 and the effective boson mass comparable with the

mass of fermions [5,8]. H^F_{eff} part, on the other hand, is given as $H^F_{eff} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} U_{\mathbf{k},\mathbf{p},\mathbf{q}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{p}\downarrow} c_{\mathbf{q}\downarrow} c_{\mathbf{k}+\mathbf{p}-\mathbf{q}\uparrow}$. Renormalization of $\varepsilon_{\mathbf{k}}$ with respect to the initial dispersion $\varepsilon^0_{\mathbf{k}}$ takes place mainly around $\mathbf{k}_F$. There is also induced the long range fermion-fermion interaction $U_{\mathbf{k},\mathbf{p},\mathbf{q}}$ which has somewhat unusual resonant-like character as shown in Figs 7 and 8 of [8] for the BCS $U_{\mathbf{k},-\mathbf{k},\mathbf{q}}$ and for the density-density $U_{\mathbf{k},\mathbf{q},\mathbf{q}}$ channels.

Previously [8] we discussed the fermion spectrum only on a basis of the quasiparticle energy $\varepsilon_{\mathbf{k}}$. However, in some cases, a considerable influence may also arise from the fermion-fermion interactions. These interactions are in principle small, $|U_{\mathbf{k},\mathbf{p},\mathbf{q}}|$ is of the order v^2, so we can treat them perturbatively. The effective dispersion $\overline{\varepsilon}_{\mathbf{k}\sigma}(l)$ is for $T > T_c$ given by

$$\overline{\varepsilon}_{\mathbf{k}\uparrow} = \varepsilon_{\mathbf{k}} + \frac{1}{N} \sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{q},\mathbf{q}} \left\langle c^\dagger_{\mathbf{q}\downarrow} c_{\mathbf{q}\downarrow} \right\rangle . \quad (2)$$

At $T < T_c$ one should also consider the other contribution coming from the BCS channel $U_{\mathbf{k},-\mathbf{k},\mathbf{q}}$. We restrict our attention only to the normal phase ($T > T_c$).

In the left h.s. panel of figure 1 we show the density of fermion states $\rho(\omega) \equiv \frac{1}{N} \sum_{\mathbf{k}} \delta(\omega - \overline{\varepsilon}_{\mathbf{k}})$. Note, that there appears a pseudogap which deepens with a decreasing temperature T. The pseudogap structure has a clear particle-hole asymmetry at all the temperatures. Asymmetry finally disappears at very high temperatures $T \simeq 0.1$ (not shown here). The boson density of states $\frac{1}{N} \sum_{\mathbf{q}} \delta(\Omega - E_{\mathbf{q}})$ is much less affected by a varying temperature (see Fig. 4 in [8]). However, upon decreasing T we observe (see the right h.s. panel of figure 1) a considerable redistribution of boson occupancy $N_B(\Omega) = \frac{1}{N} \sum_{\mathbf{q}} \delta(\Omega - E_{\mathbf{q}}) f_{BE}(E_{\mathbf{q}} - 2\mu, T)$, here f_{BE} is the Bose Einstein distribution. By comparing both the panels of figure 1 we notice that the pseudogap builds up when bosons start populating the low energy states $E_{\mathbf{q}\simeq\mathbf{0}}$.

Asymmetry of the pseudogap structure is mainly controlled by the boson concentration n_B. Here is a simple argumentation. If the boson energy is located in a center of the fermion band

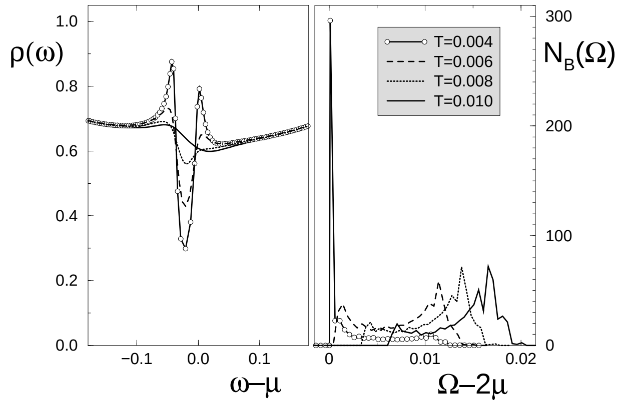

Figure 1. The density of fermion states $\rho(\omega)$ and the boson occupancy $N_B(\Omega)$ of the BF model with $v = 0.1$, $\Delta_B = 0$ and concentrations $n_F = 1$, $n_B = 0.3$. Energies ω, Ω, μ, v and $k_B T$ are all expressed in units of the femion bandwidth D.

($\Delta_B = 0$), then for the exactly half-filled fermion and boson subsystems they both must have symmetric spectra. In particular, the pseudogap would then become symmetric too. For the situation presented in Fig. 1 we have $n_F \simeq 1$, so it can only be the boson concentration n_B responsible for the asymmetry of $\rho(\omega)$. A more detailed analysis will be presented in the future publication.

4. Single particle spectroscopy

Our results, in particular effects of the particle-hole asymmetry, can be well illustrated by calculating the single particle tunneling current J. The differential conductance $\sigma(V) = dJ/dV$ as a function of bias voltage V is a direct probe of the density of states below and above the Fermi energy. We use the following expression for the STM current

$$J(V) = const \int_{-\infty}^{\infty} d\omega \; \rho(\omega) \; \left[f_{FD}(\omega, T) - f_{FD}(\omega - eV, T) \right], \quad (3)$$

where f_{FD} stands for the Fermi Dirac distribution. As usually, we neglect the energy ω and $\mathbf{k}$-dependence of the tunneling matrix [14].

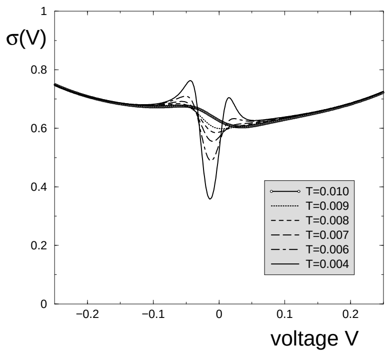

Figure 2. The STM current conductance $\sigma(V)$ as a function of bias voltage V (in units of D/e) for the same set of parameters as shown in Fig. 1.

In figure 2 we show the conductance $\sigma(V)$ of the STM current (3) obtained for the same set of parameters as in Fig. 1. We obtain the negative-positive asymmetric characteristics because, at low T, the conductance is roughly proportional to the density of states $\rho(\omega)$. Our results agree very well with the experimental data reported by Renner *et al* [15]. Unfortunately, we are unable to pass through T_c (we solve the flow equations using the one dimensional tight binding dispersion $\varepsilon^0_{\mathbf{k}}$ [8] when $T_c^{dim=1} = 0$). However, for the realistic $dim > 2$, we expect the asymmetry to survive even at $T < T_c$ as seen experimentally [15].

Let us point out the main features of the pseudogap probed experimentally by the STM conductance [15]: (i) it is asymmetric, (ii) its magnitude (the peak to peak distance) is almost temperature independent, and (iii) the pseudogap deepens with a decreasing temperature while the coherence peaks gradually start to appear. The BF model is capable to reproduce all these features (i)-(iii). Some other theoretical concepts discussed in the literature to explain $\sigma(V)$, e.g. [14] and references cited therein, are dealing with the physics which microscopically is very close to the BF model (1).

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